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# Modelling of 2D Photonic Crystals with Liquid Crystal Infilling

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## ABSTRACT

This paper presents 2D Finite Difference Time Domain (FDTD) and Finite Element (FE) modeling of Liquid Crystal (LC) devices. The enhancements to standard FDTD required for fully non-diagonal tensor materials such as LCs are outlined and they have been implemented in an in-house code. The results have been validated against a commercial FE package and good agreement is observed. The codes are then used to study in-filling of Photonic Crystal devices, in particular a benchmark structure being used a part of the COST P11 activity is used. Results are shown for transmission through the device and the effects of LC in-filling and director field rotation are seen.

## 1. INTRODUCTION

Photonic Crystal (PhC) based devices are maturing as a technology with a number of research groups and companies worldwide fabricating devices with many different functions. As with conventional integrated optics technology there is a strong requirement for tunability in these devices. There are a number of approaches that can be taken to this including thermal [1], carrier injection, Quantum Confined Stark Effect and Liquid Crystal infiltration [2]. This paper is concerned with the last of these techniques. It has long been felt that the PhC platform is ideally suited to infiltration [2] since it is normally fabricated from arrays of air holes, this coupled with the fact that LC is a well understood optical material makes this combination an interesting one. Whilst both PhC and LC based devices have been extensively modelled, the combination has received less attention [3-7]. The main reason for this is that LCs require fully non-diagonal dielectric tensors which are not normally available in commercial Electromagnetic Modelling codes used to model PhCs. This paper will use both the Finite Difference Time Domain and Finite Element methods and it will describe the enhancements required to standard FDTD required to model LCs. The paper goes on to show initial results for LC infilling of a benchmark structure being used as part of the COST P11 Photonic Crystal activity [8, 9].

## 2. MODELLING

The FDTD method has been extensively used to model PhC devices. In its standard form it can only deal with isotropic dielectric material. This can be extended reasonably easily to diagonally anisotropic material, however, fully non-diagonally anisotropic material is not so straightforward. Standard FDTD uses Maxwell's two Curl equations, in order to model fully non-diagonal tensor material the Electric Flux Density,  $\underline{D}$  is introduced into the equations as shown in equations 1 to 3.

$$\frac{\delta \underline{H}}{\delta t} = -\frac{1}{\underline{\mu}} \nabla \times \underline{E} \quad (1)$$

$$\frac{\delta \underline{D}}{\delta t} = \nabla \times \underline{H} \quad (2)$$

$$\underline{D} = \underline{\epsilon}_0 [\underline{\epsilon}_r] \underline{E} \quad (3)$$

where:

$$[\underline{\epsilon}_r] = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{bmatrix} \quad (4)$$

Now by inverting the dielectric tensor equation 4 is obtained

$$\underline{E} = [\underline{\kappa}] \underline{D} \quad (5)$$

where:

$$[\underline{\kappa}] = [\underline{\epsilon}]^{-1} \quad (6)$$

It can now be seen that we can perform field updating as in standard FDTD starting from equation 1 to give  $\underline{H}$ , equation 2 gives  $\underline{D}$ , finally equation 4 gives updated  $\underline{E}$ . This new algorithm was incorporated into our existing in-house FDTD codes [10] and validation was performed as outlined in the results section.

### 3. RESULTS

#### 3.1 Validation

In order to validate the updated FDTD codes a commercial FE simulator, COMSOL Multiphysics was used. The frequency domain option was used for these results and in this package tensor dielectrics can be specified directly. It should be pointed out here that real PhC-LC infilling requires full 3D modelling, this is because the LC can take on complex director fields within the holes and this can only be modelled in 3D. Methods such as FDTD are ideally suited to 3D modelling since they tend to scale linearly with problem size, whereas FE methods in 3D can be very slow. Thus whilst we can validate the method in 2D, validation in 3D will be more problematic.

A simple structure was used for validation purposes, this was a  $1 \times 1 \mu\text{m}$  block of material as shown in figure 1.

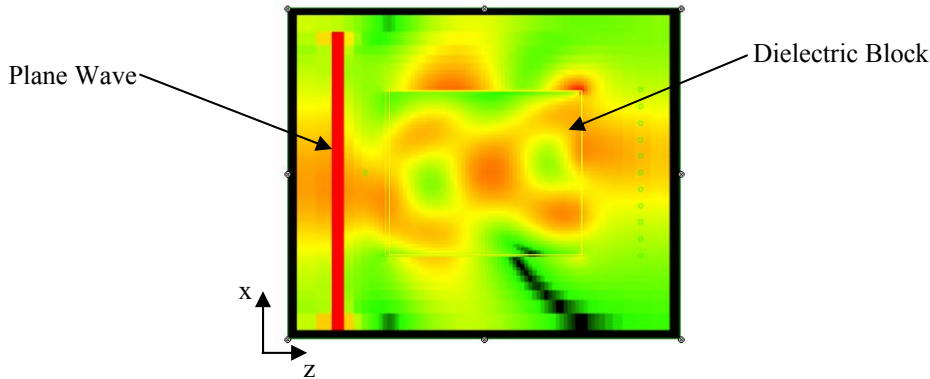


Figure 1. FDTD model of  $Abs(E_x)$  at  $1.7 \mu\text{m}$  wavelength for  $1 \times 1 \mu\text{m}$  block of material with  $\epsilon_{xx} = 9$ ,  $\epsilon_{xz} = \epsilon_{zx} = 2$ ,  $\epsilon_{zz} = 3$ .

The block is illuminated by a plane wave from the left hand side and the figure shows results obtained using Fourier Transforms for  $Abs(E_x)$  at  $1.7 \mu\text{m}$ . Spatial walk-off is observed as expected for these kind of materials, though it should be pointed out the parameters used are far from realistic. The same structure was modelled using the FE method and is shown in figure 2. It can be seen that very similar results are observed (this is more obvious in colour), the main reason for small differences are that in the FE model the plane wave is at the model edge, where as in FDTD is it within the model domain. It was felt that this level of agreement was sufficient to enable PhC modelling to be undertaken. More detailed validation will be the subject of future work.

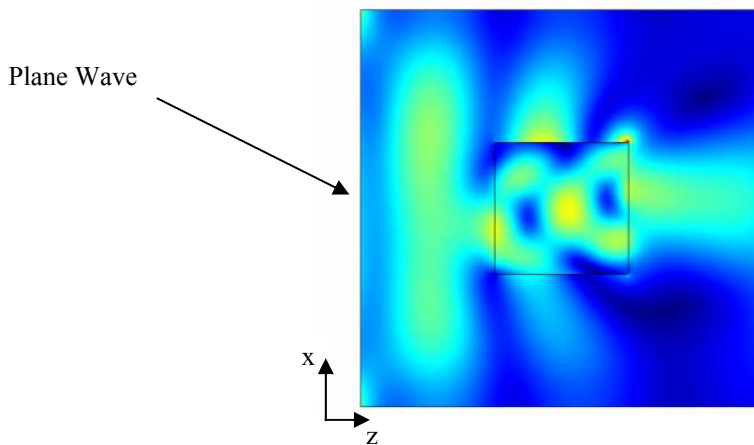


Figure 2. FE model of  $Abs(E_x)$  at  $1.7 \mu\text{m}$  wavelength for  $1 \times 1 \mu\text{m}$  block of material with  $\epsilon_{xx} = 9$ ,  $\epsilon_{xz} = \epsilon_{zx} = 2$ ,  $\epsilon_{zz} = 3$ .

#### 3.2 Photonic Crystal Infilling

Here the benchmark structure for the COST P11 modelling task [8] was used to study effect of LC infilling. Figure 3 show the structure to be studied.

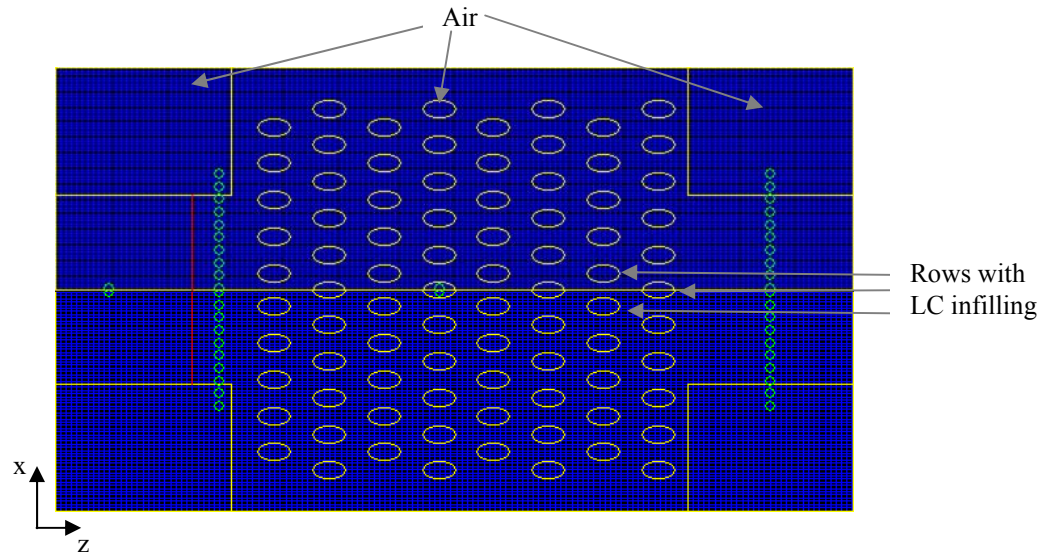


Figure 3. PhC structure to be studied with lattice constant,  $a = 230$  nm,  $r = 66$  nm,  $r/a = 0.287$  aligned in the  $\Gamma$ -M direction with background  $n = 3.38$ .

The uniform PhC is illuminated from a line source in a photonic wire input waveguide. The circular probe points are used to calculate input and output power and a reference straight waveguide simulation is used to calculate the transmission through the structure. The central line shows the plane of mirror symmetry used to reduce computation time. Figure 4 shows the transmission results obtained with air filled holes and the characteristic band gap is observed. LC is then incorporated in some of the holes. In this case we are only filling the central three rows of holes as marked on the diagram. Figure 5 shows results for LC with  $\epsilon_{xx} = 1.4$  and  $\epsilon_{zz} = 1.5$  (Diagonal) and also the case when  $\epsilon_{xx} = 1.475$ ,  $\epsilon_{zz} = 1.426$ ,  $\epsilon_{xz} = \epsilon_{zx} = 0.354$  (Off-Diagonal) which corresponds to a  $30^\circ$  rotation of the director field [3]

It can be seen that inclusion of the LC shifts the band gap slightly as expected and rotation of the director field induced a further, smaller shift. These results will also be validated using the FE codes. Extensive measurements have been carried out on these structures [9, 11] and these will be compared in detail with these results. This will ultimately require a move to full 3D modeling and the LC codes are fully 3D compatible. In fact a scheme is used based on what are called “map” files where each FDTD cell can have a different director field specified within it. Thus very complex director fields can be built up using this approach.

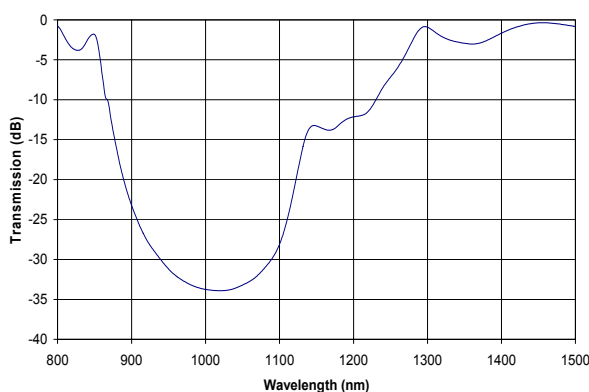


Figure 4. Transmission through structure shown in figure 3 with no LC infilling.

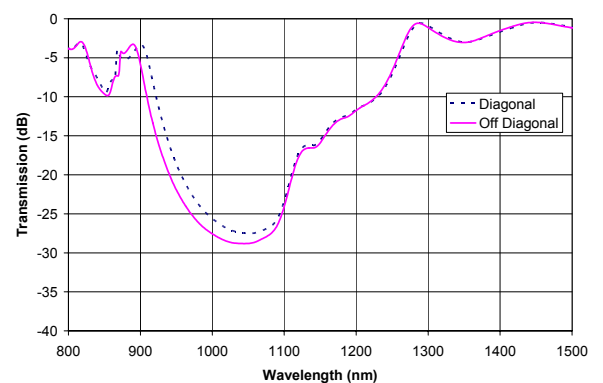


Figure 5. Transmission through structure shown in figure 3 with LC infilling in central 3 rows with diagonal and off-diagonal dielectric material.

#### 4. CONCLUSIONS

The paper presents details of a FDTD code for use with LC materials that require non-diagonal dielectric tensors to properly describe them. The code has been validated against a commercial 2D FE package. Preliminary results are then shown for LC in-filling of a PhC structure which is being used as part of a benchmarking

exercise in COST P11 and effects of director field rotation are observed. Full 3D modelling will now be pursued which will enable detailed comparison with measured results. This will enable effects such as polarisation rotation and losses to be studied in detail.

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